2-(1-Hydroxy-1-methylethyl-2-methyl-1,3-dioxane
39239-96-8 | DTXSID80192497

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 1.16

Global applicability domain: Inside

Local applicability domain index: 4.86e-01

Confidence level: 6.79e-01

Nearest Neighbors from the Training Set

Image not found
Ethanol, 2-(1,1-dimethylethoxy)-
Measured: 0.39
Predicted: 6.54e-01

Image not found
2-(Hexyloxy)ethanol
Measured: 1.86
Predicted: 1.74

Image not found
Methyl pivalate
Measured: 1.83
Predicted: 1.76

Image not found
Ethylene glycol monoisobutyl ether
Measured: 0.75
Predicted: 6.34e-01